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THE MODAL AEROSOL DYNAMICS MODEL

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Introduction

The Modal Aerosol Dynamics (MAD) model is a computationally efficient model for solving the General Dynamics Equation of Aerosols (GDE) (Friedlander, 1977). The simplifying assumption in the model is that aerosol size distributions can be approximated by overlapping modes, each represented by a continuous analytical distribution function. The development of the model for atmospheric aerosols makes use of log-normal distribution functions (LNDFs), because they reasonably represent experimental data (Whitby, 1978). This paper describes the solution of the coagulation and gas-to-particle conversion (without nucleation) terms of the GDE using the MAD model.

Coagulation

The integrals associated with coagulation in the GDE are of the form

$$\frac{dN}{dt}_i = -\frac{1}{1+\delta_{ij}} \int_0^{+\infty} \int_0^{+\infty} \beta(Dp_1, Dp_2)\, n_i(Dp_1)\, n_j(Dp_2)\, dDp_1\, dDp_2 \qquad (1)$$

where

β = collision frequency function [cm^3(air)/(#·sec)]
Dp_1, Dp_2 = Particle 1, 2 diameter [μm]
n_i, n_j = number distribution function for mode i, j
δ_{ij} = Kronecker delta function (0 for $i \neq j$, 1 for $i = j$).
N_i = Total number concentration of mode i.

The Kronecker delta is used to distinguish between intra-modal and inter-modal coagulation.

Eq (1) can be paramaterized as follows.

$$\frac{dN}{dt}_i = -K^N_{ij} N_i N_j \,. \quad K^N_{ij} = \text{number coag. coefficient} \qquad (2)$$

where

$$K^N_{ij} = \frac{1}{(1+\delta_{ij})N_i N_j}\left[\int_0^{+\infty}\int_0^{+\infty}\beta(Dp_1, Dp_2)n_i(Dp_1)\ n_j(Dp_2)\ dDp_1\ dDp_2\right] \quad (3)$$

The change in N is, therefore, a function of an equivalent coagulation coeffient (which depends on the shape of the interacting modes) and N for each mode. For LNDFs the shape of each mode is often characterized by the geometric mean size (D_g) and geometric standard deviation (σ_g). Thus, the time dependence of 3 parameters (i.e. D_g, σ_g, and N) for each mode must be calculated to track the evolution of the entire distribution. In this work, however, it is more useful to characterize the shape of each mode by the number mean surface area and volume (S/N and V/N), so the 3 parameters that are tracked are N, S, and V.

Additional equations are, therefore, formulated for changes of S, and V (V_i changes for inter-modal coagulation). For coagulation, these integrals express the change in surface area and volume for each collision and are expressed in parameterized form (K^S_{ij} and K^V_{ij} are also functions of S/N and V/N) as

$$\frac{dS}{dt}i = -K^S_{ij} N_i N_j \ . \quad K^S_{ij} = \text{surface area coag. coefficient} \quad (4)$$

$$\frac{dV}{dt}i = -K^V_{ij} N_i N_j \ . \quad K^V_{ij} = \text{volume coag. coefficient} \quad (5)$$

Gas-To-Particle Conversion

For gas-to-particle conversion (in the absence of nucleation) the primary effect is to increase aerosol volume without changing aerosol number concentration. The rate of change of modal volume concentraton is expressed as

$$\frac{dV}{dt}i = \int_0^{+\infty} \frac{dv}{dt}i\ n(v_i, t)\ dDp \quad (6)$$

where

$dv_i/dt = f(D_p)\ g(t, T, P, \text{etc.})$ = single particle growth law

v_i = single particle volume concentration

n = distribution function

V_i = modal volume concentration.

The expression for the single particle growth law depends on the mechanism of gas-to-particle conversion, and generally

depends on particle size and other physical quantities such as temperature (T), pressure (P), diffusion coefficients of condensing species, heterogeneous reaction rates, etc. Because the above integral is evaluated over the size distribution, all of the terms in dv_i/dt that are independent of Dp are taken outside of the integral and represented as g(t,T,P,etc.). The resulting expression is

$$\frac{dV}{dt}i = g(t,T,P,etc.) \int_0^{+\infty} f(D_p)\, n(v_i,t)\, dDp \qquad (7)$$

The parameterization of Eq (7) follows in an analogous manner as the parameterization of Eq (1). The result is

$$\frac{dV}{dt}i = g(t,T,P,etc.)\, C_i^V\, N_i \qquad (8)$$

where C_i^V represents the parameterization of Eq (7).

The change in S due to gas-to-particle conversion is (N does not change)

$$\frac{dS}{dt}i = \frac{dV}{dt}i\, C_i^S \qquad (9)$$

where

$$C_i^S = g(t,T,P,etc.) \left[\int_0^{+\infty} f(D_p) \frac{ds}{dv}\, n(v_i,t)\, dDp \right] \Big/ \frac{dV}{dt}i \quad . \qquad (10)$$

Combined Coagulation and Condensation

The equations for combined coagulation and gas-to-particle (g→p) conversion for a bi-modal distribution (nuclei (n) and accumulation (a) mode), are

NUCLEI MODE

$$\frac{dN}{dt}n = - K_{nn}^N N_n^2 - K_{na}^N N_n N_a \qquad (11)$$

$$\frac{dS}{dt}n = - K_{nn}^S N_n^2 - K_{na}^S N_n N_a + \left[\frac{dV}{dt}n\right]_{g\to p} C_n^S \qquad (12)$$

$$\frac{dV}{dt}n = - K_{na}^V N_n N_a + \left[\frac{dV}{dt}n\right]_{g\to p} . \qquad (13)$$

ACCUMULATION MODE

$$\frac{dN}{dt}a = - K_{aa}^N N_a^2 + K_{na}^N N_n N_a \qquad (14)$$

$$\frac{dS}{dt}a = - K^S_{aa} N_a^2 + K^S_{an} N_n N_a + \left[\frac{dV}{dt}a\right]_{g\to p} C^S_a \quad (15)$$

$$\frac{dV}{dt}a = K^V_{na} N_n N_a + \left[\frac{dV}{dt}a\right]_{g\to p} . \quad (16)$$

Comparison of the MAD Model to other Models

For simulations of pure coagulation, N, S, and V from the MAD model are within 5% of an accurate numerical solution of the GDE (Suck and Brock, 1979) and the shape of the distribution (the average mean difference between the MAD representation and an accurate numerical solution) is within 25% for all cases tested. For simulations of pure condensation N, S, and V are within 5% and the distribution shape is within 20% of an accurate numerical solution (Tsang and Brock, 1983) for all cases tested. Computational times are a factor of 1000 faster than accurate numerical solutions, and a factor of 100 faster than a sectional technique (Warren and Seinfeld, 1985) of comparable accuracy (a coarse sectionalization was chosen that yielded about the same accuracy as the MAD model). Refer to Seigneur et al, 1985, for detail on these comparisons.

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